SciDAC Allocation Request for High-Precision Heavy-Quark Physics

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for the HPQCD Collaboration

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Researchers

The HPQCD Collaboration is a collaboration of collaborations focused on achieving few-percent precision in a wide range of lattice calculations, with an emphasis on systems containing heavy quarks (Bs, Ds, Υs and ψs). The collaboration currently involves groups from Cambridge, Cornell, Fermilab, Glasgow, Illinois, Indiana, Ohio State, Simon Fraser University, Southern Methodist University, and TRIUMF. The work described in this proposal will be carried out by the following subset of the collaboration:

- Cambridge Ron Horgan (PI), and one student;
- Cornell Peter Lepage (PI), and two students;
- Ohio State Junko Shigemitsu (PI), M. Wingate (postdoc), and one student;
- Glasgow Christine Davies (PI), E. Follana and S. Collins (postdocs) and 2 students;
- Southern Methodist University Kent Hornbostel (PI);
- Simon Fraser University Howard Trottier (PI) and two students;
- TRIUMF Richard Woloshyn (PI).

The number of students involved is approximate; it cannot be predicted exactly at this time.

Allocation Request

We request 60×128 node-days of processor time on the Fermilab cluster during the next year. (This estimate, like all that follow, is for the fast nodes at Fermilab.) The Fermilab cluster is the most appropriate for two reasons. First we will be sharing large numbers of light-quark propagators with other components of the HPQCD collaboration, including the Fermilab group. Second, more than half of our processor time will be required for computing NRQCD-type propagators and evaluating two-loop perturbation theory diagrams, both of which are most efficiently done on clusters.

Scientific Program

Our goal is few-percent accurate calculations of the spectra, decay constants, mixing amplitudes, and form factors of Bs, Ds, Υs and ψs using the following ingredients:

- the MILC collaboration's existing $n_f = 3$ unquenched configurations at $a = 1/8\,\mathrm{fm}$ and $a = 1/11\,\mathrm{fm}$;
- improved staggered quark propagators for light valence quarks;
- NRQCD and moving NRQCD propagators, through order $1/M^2$, for heavy valence quarks;
- perturbatively improved currents, through order α_s^2 and $1/M^2$.

These results will have an immediate impact on heavy-quark physics since the target precision is almost an order of magnitude better that what is currently available. In particular, there are several D meson properties that can be predicted before they are measured (with comparable precision) by CLEO-c.

HPQCD, working with the MILC collaboration, has already demonstrated that high-precision results are feasible using the MILC configurations: we have demonstrated 2–5% accuracy in calculations of the upsilon spectrum, elements of the B, ψ, and light baryon spectra, and the pion and kaon decay constants — nine quantities in all so far, with no free parameters. A new determination of $\alpha_s(M_Z)$ has also been completed, and the result agrees with the current world average to within perturbative errors of $\pm 3\%$.

This feasibility study addressed three critical systematic errors. First it showed that finite lattice spacing errors, including "taste-changing" effects in improved staggered quarks, are no larger than a few percent on the finer MILC lattices. Second, it showed that the MILC quark masses are sufficiently small for reliable chiral extrapolations to physical u and d masses, again with final errors of order a few percent or less. Finally, MILC results already demonstrated that finite-volume effects are negligible at the few-percent level for all quark masses down to $m_s/8$, the smallest mass studied. We are currently measuring correlation times for the finer MILC lattices; correlations are negligible for the coarse lattices.

HPQCD has successfully completed (and published) preliminary studies of the B spectrum and decay constants that demonstrate the utility of improved staggered valence quarks. The MILC code was used to compute light-quark propagators and NRQCD, through order v^4, was used for the b quark. Studies are currently underway of three-point amplitudes for computing semileptonic form factors, and we are in the middle of an analysis of mixing. Codes for NRQCD through order v^6 and $1/M^3$ have been written and debugged; a code for moving NRQCD has been written and is currently being debugged. HPQCD has also made considerable progress on the perturbative calculations.

The computer allocation in this proposal is to cover three types of calculation:

- The calculation of approximately 6000 light-quark propagators for the $a = 1/11\,\mathrm{fm}$ MILC configurations: In order to tune the light quark masses we require a wide variety of masses in our light-quark propagators. We will need at least two of MILC's configuration sets, with approximate masses of $(0.4m_s, m_s)$ and $(0.2m_s, m_s)$, to allow for chiral extrapolation of the light sea quark masses. For each of these configuration sets we will need two large masses, to tune the s mass, and approximately four light masses covering the range between $m_s/2$ and $m_s/10$, to allow for chiral extrapolations of the light quark masses. Theoretical studies suggest that smaller masses require larger volumes than MILC is using, but this range of masses results in chiral extrapolation errors that are only of order 1–3%. Propagators from approximately 500 configurations are required for each mass. Based upon timings of the MILC code on the Fermilab cluster, we estimate that roughly 30×128 node-days of running at Fermilab will be required for this part of our calculation. These propagators will be generated in collaboration with the Fermilab group and their collaborators, and they will be available to the community. We will probably also do some parallel calculations for the coarser MILC lattices, but these require only about 1/5 the time.

- The computation of NRQCD and moving NRQCD propagators for a wide range of heavy-quark masses and reference frames (for moving NRQCD): Each light-quark propagator will be reused dozens of times in combination with different heavy-quark propagators in a wide range of calculations of B and D properties (decay constants, mixing, form factors at all momenta). Our recent experience indicates that the computer time required for the heavy-quark propagators is therefore comparable to that needed for the light-quark propagators; here we are requesting 20×128 node-days. NRQCD-type propagators are computed time slice by time slice on a single processor, with no need for inter-processor communication. This makes clusters the obvious choice for such work, and code design and optimization is straightforward. We do not save NRQCD propagators.

- High-order perturbation theory calculations: Two-loop lattice perturbation theory integrals are very expensive to compute. We have created a parallel version of vegas for use on a cluster. (Clusters are again ideal because inter-processor communication is minimal.) We estimate that about 1/6 of our allocation (10×128 node-days) will be used for perturbation theory.